A Short Course on the Application of Group Theory to Quantum Mechanics: Summary

Linear Spaces

A linear space, or vector space, over a field $\mathbb{F}=\mathbb{R},\mathbb{C},...$, is a set S with scalar multiplication and addition, that obeys:

- $A+B = B+A$
- $(A+B)+C = A+(B+C)$
- $\exists 0 : A+0 = A$
- $\exists B: A+B = 0$
- $\exists 1 : 1A = A$
- $(ab)A = a(bA)$
- $a(A+B) = aA+aB$
- $(a+b)A = aA+bA$

Linear independence of $\{A_i\}$ means that: $a_1A_1+a_2A_2+...+a_nA_n=0$ iff $a_i=0\ \forall i$

"A linear space S is n-dimensional if the maximum number of elements that are linearly independent from S is n."

"Any element in S can be expressed in terms of the linearly independent ones."

Subspaces S' are the span of elements selected from S. Subspaces have $\dim < n$.

Discrete Delta Functions

The Kronecker Delta is:

$$\delta_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases}$$

The generalized Kronecker Delta is:

$$\delta_{S_iS_j} = \begin{cases} 0 & \text{if set } \{A_i\} \neq \{A_j\} \\ 1 & \text{if set } \{A_i\} = \{A_j\} \end{cases}$$

Perturbation Theory

A Hamiltonian may be expressed as the sum of an unperturbed Hamiltonian H_0 and a perturbation H':

$$H = H_0 + H'$$

Let $\psi_1, \psi_2, ...\psi_\lambda$ be λ-fold degenerate eigenfunctions of H_0 with the energy ϵ_0. In general, $H\psi = \epsilon\psi$, so let $H'\Psi = \epsilon\Psi$:

$$\Psi \approx \sum\nolimits_i a_i\psi_i \quad \text{for best fit } a_i$$

Where a_i may be found with each ψ_k:

$$\sum\nolimits_i a_i(\langle\psi_k|H'|\psi_i\rangle - \epsilon\langle\psi_k|\psi_i\rangle) = 0$$

If $\langle\psi_k|\psi_i\rangle = \delta_{ki}$, and $H'_{ki} \equiv \langle\psi_k|H'|\psi_i\rangle$:

$$\begin{vmatrix} H_{11}-\epsilon\delta_{11} & H_{12}-\epsilon\delta_{12} & \dots & H_{1\lambda}-\epsilon\delta_{1\lambda} \\ H_{21}-\epsilon\delta_{21} & H_{22}-\epsilon\delta_{22} & \dots & H_{2\lambda}-\epsilon\delta_{2\lambda} \\ \vdots & \vdots & \ddots & \vdots \\ H_{\lambda1}-\epsilon\delta_{\lambda1} & H_{\lambda2}-\epsilon\delta_{\lambda2} & \dots & H_{\lambda\lambda}-\epsilon\delta_{\lambda\lambda} \end{vmatrix} = 0$$

The roots of this equation are ϵ^j which correspond to the state $\Psi^j = \sum_i a_i^j\psi_i$.

Note that if $\lambda=1$, then $\epsilon = \langle\psi_1|H'|\psi_1\rangle$.

Lecture 1: Introduction

Groups contain distinct elements with a definite "law of combination."

For elements to be a group:

- If A, B are in the set, so is AB
- Associativity $(AB)C = A(BC)$
- Identity Element $AI = IA = A$
- Inverses $AB=BA=I$, $A^{-1}\equiv B$

In general $AB \neq BA$, but if $AB = BA$ for all A, B, then the group is Abelian. The "order" is the number of elements. "The structure of a group is specified by all ordered pairs of elements," as may be captured in a multiplication table. Two groups with 1 : 1 elements, and same law of combination, are "isomorphic".

Ex. G_2 is the order-2 group that fulfills:

	I	E
I	I	E
E	E	I

A G_2 group might act on functions f:

$$If(x) = f(x); \qquad Ef(x) = f(-x)$$

"Image pairs" are images of each other:

$$f_+ \xrightarrow{E} f_- \xrightarrow{E} f_+ \xrightarrow{E} f_- \xrightarrow{E} f_+ \xrightarrow{E} f_- \xrightarrow{E} f_+$$

For even parity functions, $Ef_E = f_E$, and for odd parity functions, $Ef_O = -f_O$.

"Selection rules" are the orthogonality relationships arising from symmetries:

$$\int_x dx\ f_E f_O = 0$$

"Expansion theorems" state "functions with no special symmetries may be expanded in terms of functions that do":

$$f(x) = f_E + f_O \text{ for } \begin{Bmatrix} f_E = \frac{1}{2}(f(x)+f(-x)) \\ f_O = \frac{1}{2}(f(x)-f(-x)) \end{Bmatrix}$$

"For more complicated groups, more complicated symmetries are possible."

A set, and in particular, a linear space, may be "spanned" by some elements:

$$S = \{a_1f_1 + a_2f_2 : a_1, a_2 \in \mathbb{F}\}$$

f_1 and f_2 are a "basis" for this set; bases are not unique. Sets that are a sum of vectors in their subspaces that are invariant under G are "reducible":

$$S = S_1 + S_2 \text{ for } \begin{Bmatrix} S_1 = \{af_1 : a \in \mathbb{F}\} \\ S_2 = \{af_2 : a \in \mathbb{F}\} \end{Bmatrix}$$

Irreducible spaces may not be reduced to two spaces of lower dimension.

Elements in sets that are "invariant," or "closed" under a group remain in the set.

Lecture 2: Matrix Reps I

"The space S is said to be invariant under a group G, if for any function f in S and for any operator A in G, the new function Af is a function in S."

On a space invariant under a group, (basis) functions stay in the space, so:

$$Af_i = \sum\nolimits_k M_{ki}^A f_k$$

M_{ki}^A are constants in matrix $M^A = [M_{ki}^A]$, where $\{f_k\}$ generates the representation. M_{ki}^A is the component of Af_i along f_k:

$$M_{ki}^A = \langle f_k|A|f_i\rangle$$

Invariant spaces have square matrices. Here, f_k belongs to the k^{th} row and f_i belongs to the i^{th} column of the matrix.

"There is one matrix for each operator in the group." Call these matrices M^G.

For general functions in the basis $\{f_i\}$:

$$Af = A\sum\nolimits_i a_if_i = \sum\nolimits_i\sum\nolimits_k a_i\,M_{ki}^A\,f_k$$

Matrix representations in other bases:

$$\overline{M}^A = S^{-1}M^AS$$

Where S is the matrix of the new basis vectors in terms of the old basis vectors.

To find the M^A for $A \in G$ over space S:

- Choose a basis for the space S
- Act A on each basis element f_i
- The i^{th} column of M^A is Af_i

To find the transformation matrix S:

- Select an old and a new basis
- Represent each new basis element in terms of the old basis elements
- The i^{th} column of S is the i^{th} new basis element in the old basis

---

Ex. noting that $E^2 = I \Rightarrow (M^E)^2 = [\delta_{ij}]$, with an image pair $\{f_+, f_-\}$ it is found:

$$\begin{Bmatrix} If_+ = f_+ \\ If_- = f_- \end{Bmatrix} \implies M^I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\begin{Bmatrix} Ef_+ = f_- \\ Ef_- = f_+ \end{Bmatrix} \implies M^E = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

With the new basis $f_E = \frac{1}{2}(f_+ + f_-)$, and $f_O = \frac{1}{2}(f_+ - f_-)$, matrix reps are:

$$M^I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},\ M^E = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},\ S = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

Recalling (ir)-reducible spaces, if a space is reducible, with the appropriate choice of an ordered basis, M^A is then a block diagonal matrix for all $A \in G$.

Spenser Talkington, Winter Break 2018-2019

Lecture 3: Matrix Reps II

S_c is the matrix which transforms M^G into a completely reduced block form:

$$M_c^A = S_c^{-1} M^A S_c$$

Completely reduced forms are written as a diagonal sum over irreducible reps:

$$M_c^G = \sum_i a_i M_i^G \qquad \text{rep } M_i^G,\ a_i \text{ times}$$

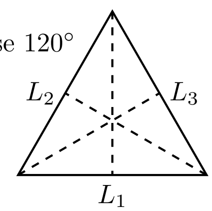
For any basis in a space with a group:

reducible space $\iff$ reducible reps

irreducible space $\iff$ irreducible reps

Ex. Order-6 group, G_6, with operators:

- I: identity
- C_r: counterclockwise 120°
- C_l: clockwise 120°
- σ_1: reflect over L_1
- σ_2: reflect over L_2
- σ_3: reflect over L_3



The group multiplication table for G_6:

	I	C_l	C_r	σ_1	σ_2	σ_3
I	I	C_l	C_r	σ_1	σ_2	σ_3
C_l	C_l	C_r	I	σ_3	σ_1	σ_2
C_r	C_r	I	C_l	σ_2	σ_3	σ_1
σ_1	σ_1	σ_2	σ_3	I	C_l	C_r
σ_2	σ_2	σ_3	σ_1	C_r	I	C_l
σ_3	σ_3	σ_1	σ_2	C_l	C_r	I

With a space spanned by the functions $\phi_i = e^{-(x-x_i)^2} e^{-(y-y_i)^2}$, corners $i = 1, 2, 3$. The representation is reduced with:

$$S = \begin{pmatrix} 1 & 0 & 2 \\ 1 & \sqrt{3} & -1 \\ 1 & -\sqrt{3} & -1 \end{pmatrix} \implies \begin{matrix}\text{one 1D irrep} \\ \text{one 2D irrep}\end{matrix}$$

For matrix M, if $\det(M) \neq 0$ then there exists S such that $S^{-1}MS$ is unitary. If M_i^G and M_k^G are irreducible unitary representations of dim λ_i and λ_k, then:

$$\sum_{j=1}^{n} \left(M_{i,ab}^{A_j}\right)^* M_{k,a'b'}^{A_j} = \frac{n}{\lambda_i} \cdot \delta_{ik} \delta_{aa'} \delta_{bb'}$$

It follows for the r irreps of the group:

$$\lambda_1^2 + \lambda_2^2 + \cdots + \lambda_r^2 = n$$

Trace, $\mathrm{tr}(A)$, is the same in all bases. The "character" A_j, is in the rep M^G:

$$T^{A_j} = \mathrm{tr}\left(M^{A_j}\right) = \sum_k M_{kk}^{A_j}$$

Through setting $a = b$, and $a' = b'$, find:

$$\sum_{j=1}^{n} \left(T_i^{A_j}\right)^* T_k^{A_j} = n \cdot \delta_{ik}$$

Now, relations for the diagonal sum:

$$T^{A_j} = \sum_{i=1}^{r} a_i T_i^{A_j} \Leftrightarrow a_i = \frac{1}{n} \sum_{j=1}^{n} \left(T_i^{A_j}\right)^* T^{A_j}$$

Which forms the reducibility relations:

$$\text{irred: } \sum \left\| T^{A_j} \right\|^2 = n, \quad \text{red: } \sum \left\| T^{A_j} \right\|^2 > n$$

Lecture 4: Applications

An operator A is unitary if and only if:

$$\langle Af | Ag \rangle = \langle f | g \rangle$$

For representations of G : G and G', and with basis functions of S: a and a':

$$\langle f_a^G | g_{a'}^{G'} \rangle = \delta_{GG'} \delta_{aa'} c;\ c = \frac{1}{\lambda} \sum_b \langle f_b^G | g_b^G \rangle$$

Selection rules are orthogonality with decomposition into basic functions:

$$\langle f_b | Dg \rangle = \langle f_b | D_b g_b \rangle$$

Expressed with the "direct product", or the Clebsch-Gordan series:

$$M_G^{D \times g} = \sum_i a_i M_i^G$$

Transform of H under operator A_j is:

$$H^j \equiv A_j H A_j^{-1}$$

With unitary A_j the energy is the same regardless of measurement location A_j:

$$\langle \Psi | H | \Psi \rangle = \langle A_j \Psi | H^j A_j \Psi \rangle$$

The "symmetric group" is A_j such that $A_j H A_j^{-1} = H$, thence note $[H, A_j] = 0$, and space of eigenfunctions is invariant.

Degeneracies of the energy levels may either be "normal" with irreducible reps or "accidental" with reducible reps.

"Barring accidents, the degree of degeneracy will correspond to the dimensions of the irreps ... furthermore, the eigenfunctions are the basic functions."

Perturbations H' that are invariant under either the symmetric group of H_0, or a subgroup of the symmetric group may be simplified using group theory.

The determinantal equation for E', $|H' - E'I| = 0$ reduces to a product:

$$|H' - E'I| = \prod_i |v_{cc'}^i - E'I|^{\lambda_i} = 0$$

$$v_{cc'}^i = \langle \Psi_n^{ic} | \Psi_n^{ic'} \rangle \text{ for } n \in \{1, 2, ..., a_i\}$$

The energies E' are the deviations from the unperturbed E, and degeneracies are predicted from dimension of irreps.

The elementary particles arise from the successive perturbations of a specific H.

Operators in continuous groups are constructed from a set of "generators." Generators are constrained by a set of structure consts: $[G_i, G_k] = \sum_j C_{ik}^j G_j$

Invariant operators are: $[A, G_i] = 0,\ \forall i$

generator $\iff$ conserved quantity

invariant op. $\iff$ observable quantity

intentionally left blank